Charge Transfer Salts of Benzene-Bridged 1,2,3,5-Dithiadiazolyl Diradicals. Preparation, Structures, and Transport Properties of 1,3- and 1,4-[(S2N2C)C6H4(CN2S2)][X] (X = I, Br)

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Table S1 Crystal and refinement data

compound	[3][I]*	[1][Br] (R = H)	[4][Br]	[3][Br]
formula	$S_4N_4C_8H_4I$	S_2N_2CHBr	$C_8H_4N_4S_4Br$	$C_8H_4N_4S_4Br$
fw	411.29	185.06	364.29	364.29
crystal size, mm	0.40 x 0.12 x 0.62	0.18 x 0.30 x 0.34	0.52 x 0.26 x 0.14	0.16 x 0.34 x 0.36
crystal color	black	red	black	black
crystal mount	on glass fiber by epoxy	in capillary with epoxy	in capillary by epoxy	on fiber with silicone glue
a, Å	28.12(1)	7.0375(7)	10.553(9)	5.649(4)
b, Å	3.487(3)	8.375(3)	16.382(3)	25.777(2)
c, Å	12.28(2)	8.883(2)	7.113(2)	16.560(9)
β, deg		103.58(2)	112.13(6)	95.79(5)
V, Å^3	1204(2)	508.86	1139(1)	2399(2)
cell detn, refls	25	25	25	25
cell detn, 2θ range, deg	16-20	16 - 21	16-40	15-20
d(calcd), g cm^{-3}	2.27	2.415	2.12	2.02
space group	Ima2	P21/a	C2/c	$P2_1/c$
Z	4	4	4	8
F_{000}	787.12	351.92	715.86	1433.5
radiation	MoK_α, graphite monochromated	MoK_α, graphite monochromated	MoK_α, graphite monochromated	MoK_α, graphite monochromated
λ, Å	0.71073	0.71073	0.71073	0.71073
temp, K	293	296	293	293
linear abs coeff,mm^{-1}	3.28	8.63	4.26	4.04
diffractometer	Enraf-Nonius CAD-4	Enraf-Nonius CAD-4	Enraf-Nonius CAD-4	Enraf-Nonius CAD-4
scan technique	θ-2θ	θ-2θ	θ-2θ	θ-2θ
scan speed, deg min^{-1}	4-16 (in omega)	4-16 (in omega)	4-16 (in omega)	4-16 (in omega)
scan width, deg	1.0 + 0.35 tanθ	1.0 + 0.35tanθ	1.0 + 0.35tanθ	1.0 + 0.35tanθ
2θ range, deg	4-50	4-50	4-50	4-50
h, k, l ranges	-33,33; 0,4; -14,14	-8,8; 0,9; 0,10	0,12; -19,19; -8,8	6,6; 0,30; 0,19
exposure time, hrs	15.5	13.6	21.3	47.6
std refl indices	-1,-1,3; 0,2,1; 0,4,0	-3,1,2; 2,-3,-1; 0,0,4	5,3,-3; 1,-5,-2; -1,5,2	2,0,2; 1,2,-5; 0,7,4
drift of stds, %	1.4	1.3	1.1	1.9
absorption correction	analytical	empirical psi scans	empirical psi scans	empirical psi scans

absorption, range	0.44-1.00	0.8529-0.9961	0.64-1.00	0.50-1.00
refl meas	2140	1858	2078	4679
unique refls	574	892	1008	4224
R for merge	0.065	0.031	0.028	0.076
data with $I > 3\sigma(I)$	336	679	786	1483
solution method	Direct Methods	SHELX	Direct Methods	Direct Methods
parameters refined	70	55	81	187
$R(F^2)$, $R_w(F^2)$[a]	0.057, 0.081	0.043, 0.064	0.033, 0.075	0.074, 0.103
GOF	1.49	1.13	1.37	1.58
p, $w^{-1}=[\sigma^2(I)+pI^2]/4F^2$	0.05	0.05	0.05	0.05
largest Δ/σ	0.007	0.000	0.000	0.000
extinction correction	none	none	108(85)[b]	
final diff map, e Å^{-3}	-0.5(1), +0.4(1)	-1.2(3),+0.5(3)	-0.51(9), +0.47(9)	-0.81(18), +1.01(18)
programs	NRC386[c]	NRC386[c]	NRC386[c]	NRC386[c]
scattering factors	Internat. Tables for Crystallography (Vol 4)		Internat. Tables for Crystallography (Vol 4)	
H atom treatment	idealized positions d(C-H) = 0.95Å	idealized positions d(C-H) = 0.95Å	idealized positions d(C-H) = 0.95; U = U_C + 0.01	idealized positions C-H = 0.95Å; U = U_C + 0.01

[a] $R = [\Sigma||F_o| - |F_c||]/[\Sigma|F_o|]$; $R_w = \{[\Sigma w||F_o| - |F_c||^2]/[\Sigma(w|F_o|^2)]\}^{1/2}$

[b] Larson, A.C., in *Crystallographic Computing*, edited by F.R. Ahmed, p. 291, 1970, Copenhagen, Munksgaard.

[c] A PC version of NRCVAX, an interactive program system for structure analysis; see E.J. Gabe, Y. LePage, J.P. Charland, F.L. Lee, and P.S. White, *J. Appl. Cryst.* **22**, 383 (1989).

*Special Note: Isotropic temperature factors of N1, N2, C1, C2, and C3 were refined independently, but the subsequent anisotropic distortions of these temperature factors were linked to reduce the number of parameters refined. Iodine position occupancies were determined during isotropic refinement and locked at those values prior to anisotropic refinement.

J6888-M3

Table S2 Atomic parameters x, y, z and B_{eq}/B_{iso} for **[4]**[I] and **[3]**[I]. ESDS refer to the last digit printed.

[4][I]

	x	y	z	B_{eq}/B_{iso}	*occupancy*
I1	0	0	0	7.70(19)	0.472
I2	0.225	0	0	7.9 (4)	0.221
I3	0.500	0	0	5.8 (5)	0.104
S	0	0.10269(5)	0.19337(3)	3.05(3)	1.0000
N	0	0.11573(20)	0.28955(12)	2.80(8)	1.0000
C1	0	0	0.32886(19)	2.21(11)	1.0000
C2	0	0	0.41657(18)	2.16(10)	1.0000
C3	0	0.11905(23)	0.45886(14)	3.10(9)	1.0000
H3	0	0.201	0.431	3.9	

[3][I]

	x	y	z	B_{eq}/B_{iso}	*occupancy*
I1	0.5000	0	1.0000	3.5 (9)	0.2466
I2	0.5000	0.5000	1.0155 (9)	4.7 (10)	0.2458
I3	0.4971 (3)	0.234 (3)	1.0070 (11)	4.3 (7)	0.2538
S1	0.88868(17)	0.1570 (17)	0.4077 (8)	5.41(23)	1.0000
S2	0.92550(17)	0.1388 (20)	0.2620 (8)	6.1 (3)	1.0000
N1	0.8370 (6)	0.123 (4)	0.3505 (12)	4.3 (3)	1.0000
N2	0.8782 (7)	0.106 (5)	0.1884 (13)	5.4 (3)	1.0000
C1	0.8389 (6)	0.090 (5)	0.2471 (14)	3.9 (3)	1.0000
C2	0.7913 (7)	0.038 (4)	0.1856 (14)	3.4 (3)	1.0000
C3	0.7921 (7)	-0.070 (5)	0.0771 (15)	3.9 (3)	1.0000
C4	0.7500	-0.133 (11)	0.0262 (15)	4.7 (13)	1.0000
C5	0.7500	0.117 (7)	0.2387 (15)	3.5 (10)	1.0000

B_{eq} is the mean of the principal axes of the thermal ellipsoid.

J6888-m4

Table S3 Interatomic distances (Å) and angles (deg) in [3][I].

Distances		Angles	
S1-S2	2.067(13)	S2-S1-N1	94.1(7)
S1-N1	1.619(18)	S1-S2-N2	94.2(7)
S2-N2	1.613(21)	S1-N1-C1	113.5(14)
N1-C1	1.276(23)	S2-N2-C1	112.8(14)
N2-C1	1.32(3)	N1-C1-N2	125.2(18)
C1-C2	1.55(3)	N1-C1-C2	117.3(16)
C2-C3	1.39(3)	N2-C1-C2	117.5(16)
C2-C5	1.360(20)	C5-C2-C1	118.8(15)
C3-C4	1.356(22)	C5-C2-C3	122.0(17)
		C1-C2-C3	119.1(15)
		C4-C3-C2	118.3(17)
		C3-C4-C3[a]	121.5(19)
		C2-C5-C2[a]	117.3(18)

[a]Symmetry code: 1.500-x, y, z

Table S4 Anisotropic temperature factors u(i,j) * 100 for [3][I]. ESDs refer to the last digit printed.

	u11	u22	u33	u12	u13	u23
I1	3.2 (6)	3.9(7)	6.1 (5)	2.4(18)	0.0	0.0
I2	5.7 (10)	5.4(8)	6.7 (6)	4.7(18)	0.0	0.0
I3	4.5 (5)	4.4(5)	7.4 (4)	3.3(17)	0.3 (4)	1.16(25)
S1	5.20(24)	11.1(4)	4.27(18)	0.5(3)	0.53(19)	0.6 (4)
S2	5.69(24)	12.1(5)	5.55(21)	1.4(3)	2.02(25)	0.5 (5)
N1	7.5 (5)	4.7(3)	4.3 (3)	0.3(4)	1.0 (3)	-0.1 (3)
N2	8.8 (5)	6.0(3)	5.6 (3)	0.3(4)	1.0 (3)	-0.1 (3)
C1	7.0 (5)	4.1(3)	3.8 (3)	0.3(4)	1.0 (3)	-0.1 (3)
C2	6.3 (5)	3.5(3)	3.1 (3)	0.3(4)	1.0 (3)	-0.1 (3)
C3	7.0 (5)	4.1(3)	3.8 (3)	0.3(4)	1.0 (3)	-0.1 (3)
C4	8.9 (19)	7.7(19)	1.3 (8)	0.0	0.0	0.8 (13)
C5	6.9 (14)	4.0(13)	2.2 (9)	0.0	0.0	0.2 (10)

Anisotropic temperature factors are of the form:

$\exp[-2\pi^2(h^2U_{11}a^{*2} + k^2U_{22}b^{*2} + l^2U_{33}c^{*2} + 2hkU_{12}a^*b^* + 2hlU_{13}a^*c^* + 2klU_{23}b^*c^*)]$.

J6888-m5

Table S5 Atomic parameters *x*, *y*, *z* and B_{eq}/B_{iso} for [1][Br] (R = H). ESDs refer to the last digit printed.

	x	*y*	*z*	B_{eq}/B_{iso}
Br	0.24355(12)	0.42096(10)	0.34541(9)	3.20(4)
S1	0.2926 (3)	0.5313 (3)	0.68768(23)	2.92(9)
S2	0.1677 (3)	0.3141 (3)	0.65796(24)	3.00(9)
N1	0.3080 (13)	0.5416 (10)	0.8675 (8)	4.3 (4)
N2	0.1538 (12)	0.2925 (9)	0.8332 (8)	3.9 (4)
C1	0.2323 (15)	0.4137 (12)	0.9208 (11)	4.3 (5)
H1	0.234	0.409	1.029	5.1

B_{eq} is the mean of the principal axes of the thermal ellipsoid

Table S6 Interatomic distances (Å) and angles (deg) in [1][Br] (R = H).

Distances		Angles	
S1-S2	2.011(3)	S2-S1-N1	96.1(3)
S1-N1	1.577(7)	S1-S2-N2	95.7(3)
S2-N2	1.593(7)	S1-N1-C1	112.2(6)
N1-C1	1.332(13)	S2-N2-C1	112.1(7)
N2-C1	1.319(13)	N1-C1-N2	123.8(8)
C1-H1	0.959(9)	N1-C1-H1	118.5(10)
		N2-C1-H1	117.7(10)

Table S7 Anisotropic temperature factors, u(i,j)*100 for [1][Br] (R = H). ESD's refer to the last digit printed.

	u11(U)	u22	u33	u12	u13	u23
Br	5.22(6)	4.02(6)	3.13(5)	-0.01(4)	1.42(4)	-0.17(3)
S1	4.92(13)	3.35(12)	2.96(10)	-0.35(9)	1.16(9)	-0.32(8)
S2	5.14(13)	3.36(11)	3.08(11)	-0.42(9)	1.34(9)	0.08(8)
N1	7.6 (5)	6.0 (5)	3.0 (4)	-0.4 (4)	1.7 (4)	-0.6 (3)
N2	6.4 (5)	5.4 (5)	3.3 (4)	0.2 (4)	1.8 (3)	0.6 (3)
C1	7.6 (7)	6.0 (6)	3.1 (5)	1.2 (5)	1.5 (4)	0.9 (4)

Anisotropic temperature factors are of the form:

$$\exp[-2\pi^2(h^2U_{11}a^{*2} + k^2U_{22}b^{*2} + l^2U_{33}c^{*2} + 2hkU_{12}a^*b^* + 2hlU_{13}a^*c^* + 2klU_{23}b^*c^*)].$$

J6888-m6

Table S8 Atomic parameters *x*, *y*, *z* and B_{eq}/B_{iso} for **[4]**[Br] and **[3]**[Br]. ESDs refer to the last digit printed.

[4][Br]

	x	*y*	*z*	B_{eq}
Br	0	0.58350(5)	1/4	3.42(6)
S1	0.09525(17)	0.40369(8)	0.2507 (3)	2.71(8)
S2	-0.10262(15)	-0.22261(9)	0.23021(24)	2.39(8)
N1	0.1105 (5)	0.3069 (3)	0.2567 (8)	2.56(25)
N2	-0.1150 (5)	-0.1231 (3)	0.2341 (8)	2.33(24)
C1	0	0.2665 (4)	1/4	2.0 (4)
C2	0	0.1760 (4)	1/4	1.9 (3)
C3	0.1161 (6)	0.1328 (3)	0.2634 (9)	2.2 (3)
C4	0.1174 (6)	0.0493 (3)	0.2632 (9)	2.2 (3)
C5	0	0.0064 (4)	1/4	1.6 (3)
C6	0	-0.0827 (4)	1/4	1.7 (4)
H3	0.197	0.339	0.274	3.0
H4	0.199	0.479	0.275	3.0

[3][Br]

	x	*y*	*z*	B_{eq}/B_{iso}
Br1	0.3294(5)	0.53488(11)	0.09196(15)	4.73(14)
Br2	0.6514(5)	0.48694(11)	0.38587(22)	6.34(16)
S1	0.8102(10)	0.03532(23)	0.2007 (4)	3.2 (3)
S2	0.5304(10)	0.08447(22)	0.1892 (4)	3.1 (3)
S3	0.7063(9)	0.37296(24)	0.3278 (4)	3.2 (3)
S4	1.0491(10)	0.39938(24)	0.3617 (4)	3.2 (3)
S5	0.5176(13)	0.4259 (3)	0.0681 (4)	4.7 (3)
S6	0.7786(14)	0.4639 (3)	0.1347 (4)	5.2 (3)
S7	0.9417(10)	0.08602(23)	0.0306 (3)	3.1 (3)
S8	0.6128(10)	0.12072(23)	0.0034 (4)	3.1 (3)
N1	0.986 (3)	0.0745 (7)	0.2496 (11)	3.4 (4)
N2	0.667 (3)	0.1320 (7)	0.2347 (11)	3.1 (4)
N3	0.779 (3)	0.3128 (7)	0.3301 (10)	3.3 (4)
N4	1.166 (3)	0.3425 (7)	0.3674 (10)	3.1 (4)
N5	0.639 (3)	0.3713 (7)	0.0734 (11)	3.9 (4)
N6	0.954 (4)	0.4149 (8)	0.1442 (12)	4.9 (5)
N7	1.067 (3)	0.1387 (7)	0.0687 (10)	2.7 (4)
N8	0.698 (3)	0.1788 (7)	0.0351 (10)	2.9 (4)

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Table S8 (cont'd)

	x	y	z	B_{eq}/B_{iso}
C1	0.892 (4)	0.1199 (9)	0.2658 (14)	3.4 (5)
C2	1.035 (4)	0.1604 (8)	0.3117 (12)	2.5 (4)
C3	1.246 (4)	0.1467 (9)	0.3564 (13)	3.2 (5)
C4	1.381 (4)	0.1854 (8)	0.3998 (13)	3.2 (5)
C5	1.312 (4)	0.2371 (9)	0.3959 (13)	3.4 (5)
C6	1.093 (4)	0.2500 (8)	0.3562 (12)	2.4 (4)
C7	0.957 (4)	0.2110 (8)	0.3145 (13)	2.7 (4)
C8	1.018 (4)	0.3033 (9)	0.3499 (14)	3.7 (5)
C9	0.870 (4)	0.3700 (9)	0.1122 (13)	3.4 (5)
C10	0.992 (4)	0.3225 (8)	0.1213 (12)	2.5 (4)
C11	1.223 (4)	0.3224 (10)	0.1667 (15)	4.4 (6)
C12	1.339 (4)	0.2765 (8)	0.1780 (13)	3.0 (5)
C13	1.253 (4)	0.2304 (9)	0.1415 (13)	3.2 (5)
C14	1.021 (4)	0.2295 (8)	0.0990 (13)	2.9 (5)
C15	0.904 (4)	0.2763 (8)	0.0879 (13)	2.9 (4)
C16	0.924 (4)	0.1808 (8)	0.0651 (13)	2.9 (4)
H3	1.297	0.112	0.358	4.0
H4	1.531	0.176	0.427	4.0
H5	1.422	0.262	0.419	4.2
H7	0.809	0.220	0.285	3.5
H11	1.281	0.354	0.192	5.2
H12	1.492	0.276	0.208	3.8
H13	1.348	0.200	0.144	4.0
H15	0.760	0.278	0.053	3.7

B_{eq} is the mean of the principal axes of the thermal ellipsoid

J6888-MS

Table S9 Interatomic distances (Å) and angles (deg) in [**4**][Br].

Distances		Angles	
S1-S1'	2.007(4)	S1'-S1-N1	95.23(20)
S1-N1	1.593(5)	S2'-S2-N2	94.79(19)
S2-S2'	2.076(4)	S1-N1-C1	114.7(4)
S2-N2	1.637(5)	S2-N2-C6	114.5(4)
N1-C1	1.326(6)	N1-C1-N1'	120.1(6)
N2-C6	1.348(6)	N1-C1-C2	119.9(3)
C1-C2	1.482(10)	C1-C2-C3	120.7(3)
C2-C3	1.387(6)	C3-C2-C3'	118.7(6)
C3-C4	1.368(8)	C2-C3-C4	121.3(5)
C4-C5	1.396(7)	C3-C4-C5	119.6(5)
C5-C6	1.461(9)	C4-C5-C6	120.2(3)
		N2-C6-N2'	121.3(6)
		N2-C6-C5	119.3(3)

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Table S10 Interatomic distances (Å) and angles (deg) in [3][Br].

Distances

S1-S2	2.020(8)	N7-C16	1.35(3)
S1-N1	1.580(18)	N8-C16	1.32(3)
S2-N2	1.596(18)	C1-C2	1.48(3)
S3-S4	2.076(8)	C2-C3	1.39(3)
S3-N3	1.605(19)	C2-C7	1.38(3)
S4-N4	1.608(18)	C3-C4	1.41(3)
S5-S6	2.004(9)	C4-C5	1.39(3)
S5-N5	1.564(20)	C5-C6	1.38(3)
S6-N6	1.603(22)	C6-C7	1.41(3)
S7-S8	2.071(8)	C6-C8	1.44(3)
S7-N7	1.629(17)	C9-C10	1.41(3)
S8-N8	1.643(18)	C10-C11	1.43(3)
N1-C1	1.32(3)	C10-C15	1.39(3)
N2-C1	1.36(3)	C11-C12	1.36(3)
N3-C8	1.38(3)	C12-C13	1.40(3)
N4-C8	1.32(3)	C13-C14	1.42(3)
N5-C9	1.40(3)	C14-C15	1.38(3)
N6-C9	1.34(3)	C14-C16	1.46(3)

Angles

S2-S1-N1	95.2(7)	C5-C6-C7	118.9(19)
S1-S2-N2	95.8(7)	C5-C6-C8	120.6(19)
S4-S3-N3	94.6(7)	C7-C6-C8	120.2(18)
S3-S4-N4	94.8(7)	C2-C7-C6	122.0(18)
S6-S5-N5	96.6(8)	N3-C8-N4	120.0(21)
S5-S6-N6	94.8(8)	N3-C8-C6	117.5(20)
S8-S7-N7	94.0(7)	N4-C8-C6	122.4(20)
S7-S8-N8	95.5(7)	N5-C9-N6	116.1(20)
S1-N1-C1	115.3(15)	N5-C9-C10	119.7(20)
S2-N2-C1	113.0(15)	N6-C9-C10	124.0(20)
S3-N3-C8	114.8(15)	C9-C10-C11	117.9(19)
S4-N4-C8	115.8(16)	C9-C10-C15	123.6(19)
S5-N5-C9	115.5(16)	C11-C10-C15	118.5(19)
S6-N6-C9	116.7(17)	C10-C11-C12	118.5(21)
S7-N7-C16	114.6(14)	C11-C12-C13	122.3(20)
S8-N8-C16	113.4(14)	C12-C13-C14	119.5(20)
N1-C1-N2	120.3(20)	C13-C14-C15	117.2(19)
N1-C1-C2	121.4(19)	C13-C14-C16	119.7(19)
N2-C1-C2	118.1(19)	C15-C14-C16	123.0(19)
C1-C2-C3	119.2(19)	C10-C15-C14	123.3(19)
C1-C2-C7	121.7(18)	N7-C16-N8	122.5(18)
C3-C2-C7	119.0(19)	N7-C16-C14	118.1(18)
C2-C3-C4	119.0(20)	N8-C16-C14	119.3(19)
C3-C4-C5	121.5(19)		
C4-C5-C6	119.1(20)		

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Table S11 Anisotropic temperature factors, u(i,j)*100 for [**4**][Br] and [**3**][Br]. ESD's refer to the last digit printed.

[**4**] [Br]

	u11(U)	u22	u33	u12	u13	u23
Br	6.61(8)	1.89(6)	5.27(7)	0.0	3.13(6)	0.0
S1	3.38(9)	1.55(8)	5.93(12)	0.18(5)	2.41(8)	-0.29(6)
S2	2.88(8)	1.57(8)	4.92(11)	0.29(5)	1.81(8)	0.06(6)
N1	3.2 (3)	1.4 (2)	5.7 (4)	-0.27(19)	2.4 (3)	0.01(20)
N2	2.7 (3)	1.7 (2)	4.9 (3)	-0.30(18)	1.94(25)	-0.20(19)
C1	3.2 (4)	0.8 (3)	4.3 (5)	0.0	2.1 (4)	0.0
C2	3.0 (4)	1.1 (4)	2.9 (4)	0.0	0.9 (4)	0.0
C3	2.6 (3)	1.8 (3)	4.1 (4)	-0.18(22)	1.7 (3)	0.26(22)
C4	2.5 (3)	2.0 (3)	4.0 (4)	-0.52(23)	1.4 (3)	0.09(22)
C5	2.5 (4)	1.5 (3)	2.2 (4)	0.0	1.2 (3)	0.0
C6	2.0 (4)	1.7 (4)	3.0 (4)	0.0	1.2 (3)	0.0

[**3**] [Br]

	u11	u22	u33	u12	u13	u23
Br1	7.5(2)	5.6(2)	4.9(2)	0.4(2)	0.8(1)	-0.9(1)
Br2	5.6(2)	4.4(2)	13.1(3)	0.3(2)	-4.0(2)	1.5(2)
S1	3.8(4)	3.7(3)	4.4(4)	1.0(3)	-1.0(3)	0.2(3)
S2	2.7(3)	3.9(4)	4.9(4)	-0.1(3)	-1.2(3)	-0.5(3)
S3	2.0(3)	5.3(4)	4.5(4)	-0.1(3)	-1.2(3)	-0.2(3)
S4	3.2(3)	4.9(4)	3.8(4)	-1.1(3)	-0.6(3)	0.5(3)
S5	7.1(5)	3.7(4)	6.7(5)	0.3(4)	-1.6(4)	-0.5(3)
S6	8.9(5)	4.9(4)	5.7(4)	-0.6(4)	-1.6(4)	-1.1(4)
S7	3.2(3)	4.3(4)	3.8(3)	0.8(3)	-1.0(3)	-0.1(3)
S8	3.0(3)	3.6(4)	4.9(4)	0.3(3)	-1.0(3)	-0.1(3)

Anisotropic temperature factors are of the form:

$$\exp[-2\pi^2(h^2U_{11}a^{*2} + k^2U_{22}b^{*2} + l^2U_{33}c^{*2} + 2hkU_{12}a^*b^* + 2hlU_{13}a^*c^* + 2klU_{23}b^*c^*)].$$

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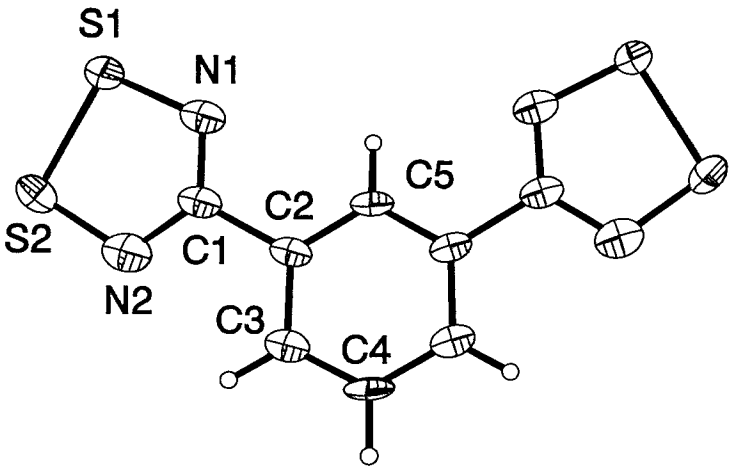
Figure S1 ORTEP drawings (30% ellipsoids) of [**3**][I] (above) and [**1**][Br] (R = H) (below).



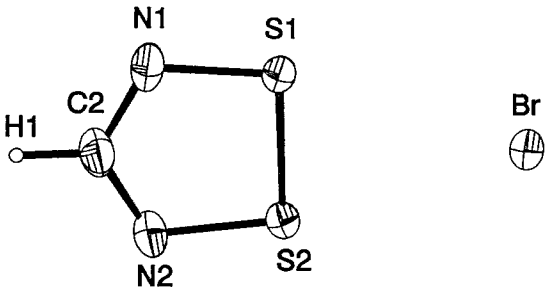


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Figure S2 ORTEP drawings (30% ellipsoids) of [**4**][Br] (above) and [**3**][Br] (below).